

PARTITION FUNCTION ZEROS OF APERIODIC ISING MODELS

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We consider Ising models defined on periodic approximants of aperiodic graphs. The model contains only a single coupling constant and no magnetic field, so the aperiodicity is entirely given by the different local environments of neighbours in the aperiodic graph. In this case, the partition function zeros in the temperature variable, also known as the Fisher zeros, can be calculated by diagonalisation of finite matrices. We present the partition function zero patterns for periodic approximants of the Penrose and the Ammann-Beenker tiling, and derive precise estimates of the critical temperatures.

1 Introduction

The Ising model is the paradigm for a second-order phase transition in two-dimensional models of statistical mechanics. Without an external magnetic field, the partition function of the two-dimensional Ising model can be calculated explicitly for regular lattices. However, if the Ising model is defined on an aperiodic graph, for instance on the Penrose tiling (PT), this is no longer the case. Therefore, the influence of an aperiodic order in the underlying structure on the phase transition of the Ising model has been investigated by various means, including numerical simulations, series expansions, and zeros of the partition function; an overview on the results and a comprehensive lists of references on the subject can be found in recent review articles.^{1,2}

The most general prediction stems from heuristic scaling arguments, adapted from a relevance criterion for disordered Ising models.² It yields an inequality involving a characteristic exponent that describes the fluctuations in the disordered or aperiodically ordered system, the correlation critical exponent ν of the pure system, and the space dimension of the fluctuation. Planar quasiperiodic graphs obtained by cut-and-project methods³ have low fluctuations, because they are flat sections through higher-dimensional peri-

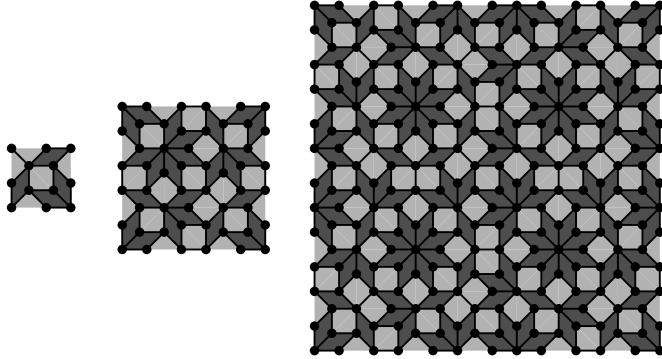


Figure 1. The first three periodic approximants ($m = 1, 2, 3$) of the Ammann-Beenker tiling.

odic lattices. Therefore, the aperiodicity is expected to be irrelevant in these cases, which conforms with the results obtained for specific examples, notably the PT.

Here, we consider partition function zeros obtained for periodic approximants of the rhombic PT and the Ammann-Beenker tiling (ABT). The unit cells of the first three approximants for the latter are shown in Fig. 1.

2 The Ising model

We place Ising spins $\sigma_{j,k} \in \{-1, 1\}$ on the vertices of the periodic approximants. Spins interact by a nearest-neighbour interaction J . The energy of a configuration $\sigma = \{\sigma_j \mid 1 \leq j \leq M\} \in \{-1, 1\}^M$ on a finite graph with M vertices is

$$E(\sigma) = - \sum_{\langle j,k \rangle} J \sigma_j \sigma_k, \quad (1)$$

where the summation is performed over all pairs $\langle j, k \rangle$ of neighbouring spins, i.e., those located on vertices that are connected by an edge. The corresponding partition function is the sum on all configurations

$$Z(\beta) = \sum_{\sigma} \exp[-\beta E(\sigma)], \quad (2)$$

where β is the inverse temperature.

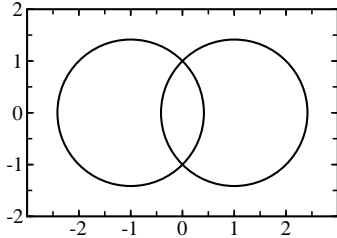


Figure 2. Partition function zeros of the square lattice Ising model.

3 Partition function zeros

We are interested in the pattern of zeros of this function in the complex temperature plane. In the thermodynamic limit $M \rightarrow \infty$, the zeros accumulate, filling curves or areas in the complex plane. These separate different regions of analyticity of the free energy, which is essentially the logarithm of the partition function, and hence correspond to phase transitions.

The zero pattern for the square lattice case is shown in Fig. 2, which displays the zeros in the complex variable $z = \exp(2\beta J)$. It consists of two circles. The two intersections at $z = \sqrt{2} + 1$ and $z = \sqrt{2} - 1$ with the positive real axis correspond to the ferromagnetic and antiferromagnetic critical points $w_c = \tanh(\beta_c J) = \pm\sqrt{2}$, respectively.

4 Results and conclusions

The partition function zeros of the Ising model on any periodic planar graph with N spins in a unit cell can be calculated by diagonalising a two-parameter family of $4N \times 4N$ matrices.^{4,5} The powerful tool behind this method is the Kac-Ward determinant or Pfaffian method for calculating the Ising model partition function on general planar graphs.⁴ Thus, this method allows to compute partition function zeros for Ising models on infinite periodic graphs with an arbitrary numerical precision.

The result for the first approximants of the PT and the ABT are shown in Figs. 3 and 4. These show accumulated zeros obtained by diagonalising the Kac-Ward matrix for various values of the two parameters, again in the complex variable $z = \exp(2\beta J)$. The corresponding values of the critical temperature are listed in Table 1. These yield precise estimates for the critical temperature for the aperiodic tilings, the errors were estimated on the basis of the apparent convergence of the first few terms.

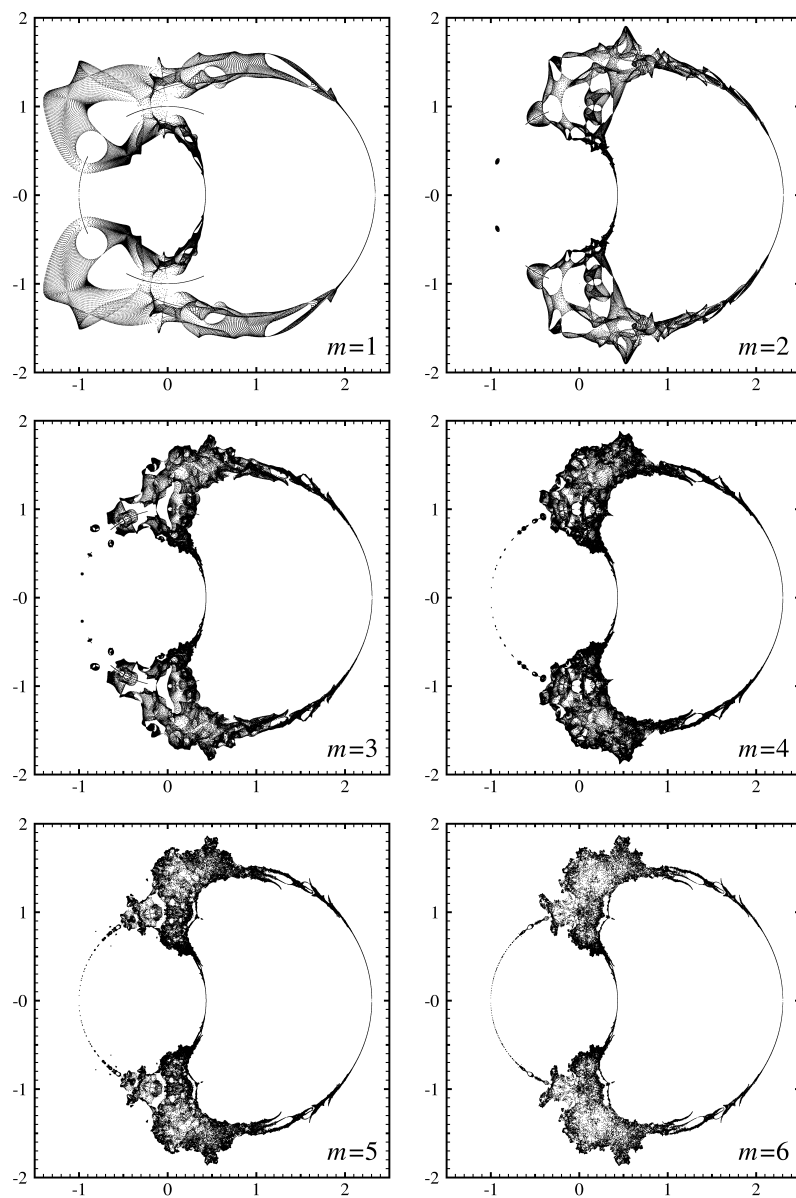


Figure 3. Part of partition function zeros for periodic approximants of the Penrose tiling.

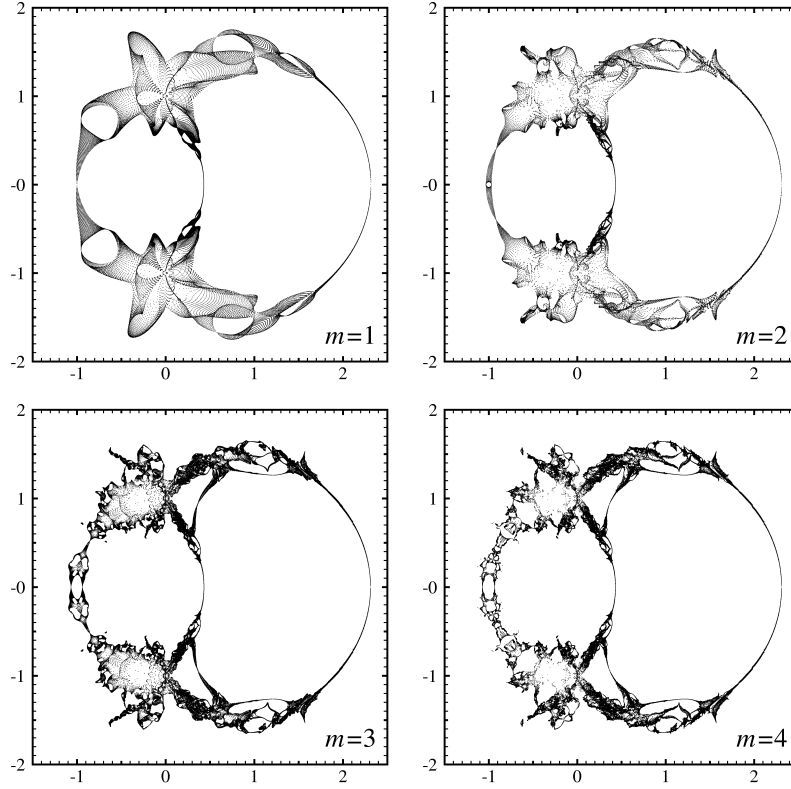


Figure 4. Partition function zeros for periodic approximants of the Ammann-Beenker tiling.

The zero patterns, besides the trivial symmetry under complex conjugation of z , still show the $z \leftrightarrow z^{-1}$ symmetry that is a consequence of the bipartiteness of the tilings. This also implies that the ferromagnetic and antiferromagnetic phase transitions are of the same type. However, some of the symmetry of the square lattice case, corresponding to the self-duality of the square-lattice Ising model, is lost. In fact, the dual graphs of the aperiodic graphs under consideration contain triangles, hence are not bipartite. The antiferromagnetic model on these dual graphs will suffer frustration. This may be responsible for the rather complicated, presumably fractal or fractally bounded zero patterns, particularly further away from the positive real

Table 1. Critical temperatures $w_c = \tanh(\beta_c J)$ for periodic approximants of the PT and the ABT. Here, m labels the approximants with N spins per unit cell.

m	<u>Penrose tiling</u>		<u>Ammann-Beenker tiling</u>	
	N	w_c	N	w_c
1	11	0.401 440 380	7	0.396 850 570
2	29	0.395 411 099	41	0.396 003 524
3	76	0.395 082 894	239	0.395 985 346
4	199	0.394 554 945	1393	0.395 984 811
5	521	0.394 523 576	8119	0.395 984 795
6	1364	0.394 454 880	47321	0.395 984 795
7	3571	0.394 451 035		
8	9349	0.394 441 450		
9	24476	0.394 439 826		
10	64079	0.394 439 319		
∞	∞	0.394 439(1)	∞	0.395 984 79(1)

axis. The zeros around the two phase transition points still lie on a circle intersecting the real axis orthogonally, consistent with the fact that the phase transition belongs to the same universality class as on the square lattice.

References

1. U. Grimm and M. Baake, Aperiodic Ising models, in *The Mathematics of Long-Range Aperiodic Order*, ed. R.V. Moody (Kluwer, Dordrecht, 1997), pp. 199–237.
2. U. Grimm, Aperiodicity and disorder - does it matter? In *Computational Statistical Physics — From Billiards to Monte-Carlo*, eds. K.-H. Hoffmann and M. Schreiber (Springer, Berlin, 2001).
3. U. Grimm and M. Schreiber, Aperiodic Tilings on the Computer, in *Quasicrystals*, eds. J.-B. Suck, M. Schreiber and P. Häussler (Springer, Berlin, 2002, to appear).
4. P. Repetowicz, U. Grimm and M. Schreiber, High-temperature expansion for Ising models on quasiperiodic tilings, *J. Phys. A: Math. Gen.* **32**, 4397–4418 (1999).
5. P. Repetowicz, U. Grimm and M. Schreiber, Planar quasiperiodic Ising models, *Mat. Sci. Eng. A* **294–296**, 638–641 (2000).